1. UMass statistics module
2. Web-based resources
3. MATLAB tools
Applied Statistics & Data Analytics

UMass Statistics Module
Background

- Sophomore level course
- Description: development and analysis of mathematical models for chemical engineering systems
- Topics: statistics for data analysis, linear and nonlinear algebraic equation models, ordinary differential equation models and numerical methods for model solution
- Statistics objective: be able to perform statistical analysis of experimental data and to use computer-based tools for data analysis
Statistics Lecture Topics: 4 Weeks

- Introduction
- MATLAB: Introduction
- Probability
- Probability distributions
- MATLAB: Manipulating data
- Binomial & normal distributions
- Confidence intervals
- MATLAB: Functions
- Hypothesis testing
- Correlation & regression analysis
- MATLAB: Statistics toolbox
- Experimental design
- MATLAB: Statistical analysis
Statistics Homeworks and Tests

- 3 written homeworks
  - Probability
  - Probability distributions; binomial, Poisson & normal distributions
  - Confidence intervals; hypothesis testing
- 1 MATLAB homework
  - Experimental design; correlation & regression analysis; response surface modeling
- 1 midterm exam
- 1 of 3 options for final project
- All materials available upon request
Applied Statistics & Data Analytics

Web-based Resources
The Probability Web

"It is remarkable that a science which began with the consideration of games of chance should have become the most important object of human knowledge."

Pierre Simon, Marquis de Laplace, Théorie Analytique des Probabilités

Welcome to the Probability Web

The Probability Web is a collection of probability resources on the World Wide Web (WWW). The pages are designed to be especially helpful to researchers, teachers, and people in the probability community.

The Probability Web was conceived and first developed by Phil Pollett at the University of Queensland. Past maintainers are:

• Phil Pollett from October 1995 to February 2001;
• Bob Dobrow from March 2001 to December 2010.

In January 2011 technical responsibility for the site was taken over by Jim Pitman with organizational and editorial support of David Aldous and Raya Feldman. We are looking for further volunteers to help distribute the editorial load and to improve the quality and scope of the site. If you are interested in assisting, if you have information, comments, or suggestions for improvement, or if you know of a probability resource on the Web that you don't see here, please contact one of the above people by email (addresses on their webpages).

Page last modified: Jan 17, 2011
Teaching Resources

The Probability Web

On-line tutorials and textbooks

- Analytical Argumentations of Probability and Statistics by Giacomo Lorenzoni
- Calculus Applied to Probability and Statistics for Liberal Arts and Business Majors, by Stefan Waner and Steven R. Costenoble
- Introduction to Probability, by Charles M. Grinstead and J. Laurie Snell
- Learning Probability Theory via Tutorial Dialogues
- Probability Theory: The Logic of Science, by E.T. Jaynes
- Probability Tutorials, Advanced probability, measure theory, by Noel Vaillant
- A Short Introduction to Probability, by Dr. Dirk P. Kroese.
- Statistiques Médicales En Ligne, Interactive probability and statistics course (in French) with many Java applets, using both real and simulated data.
- Virtual Laboratories in Probability and Statistics, Provides interactive resources for students and teachers.

Interactive demonstrations

- Cut the Knot: Probability puzzles.
- Java Demos for Probability and Statistics.
- Primordial Soup Kitchen: Cellular automata.

General resources

- Chance: A wealth of material to teach a Chance course. Laurie Snell, Dartmouth College.
Probabilistic Learning Activities Network

Welcome to planetqhe! This site is primarily written for International Baccalaureate students but can be used in any high school math class, especially those involving project work or coursework.

There are over 30 probability activities based on questions; answers are deliberately left out. That’s why planetqhe stands for Probabilistic Learning Activities: Question, Hypothesis, Experiment. There are two types of question - QHE questions relate to the activities. Essential questions bridge each set of activities.

How do I get started?

- Read teacher support for some ideas about applying planetqhe in the classroom.
- Don’t miss technology support for essential information about how to get everything working properly.
- IB teachers can see how planetqhe fits with the IB curriculum by checking this curriculum matrix.
- Queries and feedback - email planetqhe@hotmail.com. Or send me your probability anecdotes.
- Don’t forget to support this site - or visit the probability store to check out recommended books and dice.

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Virtual Laboratories in Probability & Statistics

Random

Probability, Mathematical Statistics, Stochastic Processes

Welcome!

**Random** (formerly Virtual Laboratories in Probability and Statistics) is a website devoted to probability, mathematical statistics, and stochastic processes, and is intended for teachers and students of these subjects. The site consists of an integrated set of components that includes expository text, interactive web apps, data sets, biographical sketches, and an object library. Please read the **Introduction** for more information about the content, structure, mathematical prerequisites, technologies, and organization of the project. Random is hosted at two sites: www.math.uah.edu/stat/ and www.randomservices.org/stat. For updates, please follow @randomservices on Twitter.

Technologies and Browser Requirements

This site uses a number of advanced (but open and standard) technologies, including HTML5, CSS, and JavaScript. To use this project properly, you will need a modern browser that supports these technologies. The latest versions of Chrome, Firefox, Opera, and Safari are the best choices. The Internet Explorer and Edge browsers for Windows do not fully support the technologies used in this project.

Display of mathematical notation is handled by the open source MathJax project.

Support and Partnerships

This project was partially supported by a two grants from the Course and Curriculum Development Program of the National Science Foundation (award numbers DUE-9652870 and DUE-0089377). This project is also partially supported by the University of Alabama in Huntsville. Please see the support and credits page for additional information.

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Applied Statistics & Data Analytics

MATLAB Tools
MATLAB: Statistics Toolbox

Overview
Statistics Toolbox Capabilities

- Descriptive statistics
- Statistical visualization
- Probability distributions
- Hypothesis tests
- Linear models
- Nonlinear models
- Multivariate statistics
- Statistical process control
- Design of experiments
- Hidden Markov models
Histograms

```matlab
>> y = [1 3 5 8 2 4 6 7 8 3 2 9 4 3 6 7 4 1
      5 3 5 8 9 6 2 4 6 1 5 6 9 8 7 5 3 4 5 2 9
      6 5 9 4 1 6 7 8 5 4 2 9 6 7 9 2 5 3 1 9 6
      8 4 3 6 7 9 1 3 4 7 5 2 9 8 5 7 4 5 4 3 6
      7 9 3 1 6 9 5 6 7 3 2 1 5 7 8 5 3 1 9 7 5
      3 4 7 9 1]’;
>> mean(y) → ans = 5.1589
>> var(y) → ans = 6.1726
>> std(y) → ans = 2.4845
>> hist(y,9) → histogram plot with 9 bins
>> n = hist(y,9) → store result in vector n
>> x = [2 4 6 8]’
>> n = hist(y,x) → create histogram with bin centers specified by vector x
```
Permutations and Combinations

>> perms([2 4 6]) → all possible permutations of 2, 4, 6
   6  4  2
   6  2  4
   4  6  2
   4  2  6
   2  4  6
   2  6  4

>> randperm(6) → returns one possible permutation of 1-6
   5  1  2  3  4  6

>> nchoosek(5,4) → number of combinations of 5 things taken 4 at a time without repetitions
   ans = 5

>> nchoosek(2:2:10,4) → all possible combinations of 2, 4, 6, 8, 10 taken 4 at a time without repetitions
   2  4  6  8
   2  4  6  10
   2  4  8  10
   2  6  8  10
   4  6  8  10
Probability Distributions

- 21 continuous distributions for data analysis
  » Includes normal distribution
- 6 continuous distributions for statistics
  » Includes chi-square and t distributions
- 8 discrete distributions
  » Includes binomial and Poisson distributions
- Each distribution has functions for:
  » pdf — Probability density function
  » cdf — Cumulative distribution function
  » inv — Inverse cumulative distribution
  » functionsstat — Distribution statistics function
  » fit — Distribution fitting function
  » like — Negative log-likelihood function
  » rnd — Random number generator
Normal Distribution Functions

- normpdf – probability distribution function
- normcdf – cumulative distribution function
- norminv – inverse cumulative distribution function
- normstat – mean and variance
- normfit – parameter estimates and confidence intervals for normally distributed data
- normlike – negative log-likelihood for maximum likelihood estimation
- normrnd – random numbers from normal distribution
Normal Distribution Examples

- Normal distribution: \( \text{normpdf}(x, \mu, \sigma) \)
  - \( \text{normpdf}(8,10,2) \rightarrow \text{ans} = 0.1210 \)
  - \( \text{normpdf}(9,10,2) \rightarrow \text{ans} = 0.1760 \)
  - \( \text{normpdf}(8,10,4) \rightarrow \text{ans} = 0.0880 \)

- Normal cumulative distribution: \( \text{normcdf}(x, \mu, \sigma) \)
  - \( \text{normcdf}(8,10,2) \rightarrow \text{ans} = 0.1587 \)
  - \( \text{normcdf}(12,10,2) \rightarrow \text{ans} = 0.8413 \)

- Inverse normal cumulative distribution: \( \text{norminv}(p, \mu, \sigma) \)
  - \( \text{norminv}([0.025 \ 0.975],10,2) \rightarrow \text{ans} = 6.0801 \quad 13.9199 \)

- Random number from normal distribution: \( \text{normrnd}(\mu, \sigma, v) \)
  - \( \text{normrnd}(10,2,[1 \ 5]) \rightarrow \text{ans} = 9.1349 \quad 6.6688 \quad 10.2507 \quad 10.5754 \quad 7.7071 \)
Normal Distribution Example

- The temperature of a bioreactor follows a normal distribution with an average temperature of 30°C and a standard deviation of 1°C. What percentage of the reactor operating time will the temperature be within +/-0.5°C of the average?

- Calculate probability at 29.5°C and 30.5°C, then calculate the difference:
  - \( p = \text{normcdf}([29.5\ 30.5],30,1) \)
  - \( p = [0.3085\ 0.6915] \)
  - \( p(2) - p(1) \)
  - 0.3829

- The reactor temperature will be within +/- 0.5°C of the average ~38% of the operating time.
Confidence Intervals

>> [muhat,sigmahat,muci,sigmaci] = normfit(data,alpha)
- data: vector or matrix of data
- alpha: confidence level = 1-alpha
- muhat: estimated mean
- sigmahat: estimated standard deviation
- muci: confidence interval on the mean
- sigmaci: confidence interval on the standard deviation

>> [muhat,sigmahat,muci,sigmaci] = normfit([1.25 1.36 1.22 1.19 1.33 1.12 1.27 1.27 1.31 1.26],0.05)
- muhat = 1.2580
- sigmahat = 0.0697
- muci = 1.2081
  1.3079
- sigmaci = 0.0480
  0.1273
MATLAB: Statistics Toolbox

In-class Exercise
Membrane Quality

- A membrane manufacturer sells membranes with three different pore sizes
- The average pore size of the membranes supposedly meet the following specifications (in microns):
  - Small pore membranes: $\mu = 50$, $s = 2.5$
  - Medium pore membranes: $\mu = 75$, $s = 5$
  - Large pore membranes: $\mu = 125$, $s = 10$
- The Excel spreadsheet membranes.xls contains the average pore size measured for 25 membranes of each pore size
- Determine if the specifications are satisfied to a 95% confidence level
Exercise

\[
\begin{array}{cccc}
1 & 55 & 73 & 125 \\
2 & 54 & 80 & 123 \\
3 & 55 & 74 & 118 \\
4 & 57 & 77 & 99 \\
5 & 58 & 79 & 123 \\
6 & 52 & 81 & 112 \\
7 & 51 & 80 & 121 \\
8 & 48 & 84 & 132 \\
9 & 61 & 77 & 121 \\
10 & 60 & 72 & 127 \\
\vdots & \vdots & \vdots & \vdots \\
\end{array}
\]

\[
\begin{array}{c}
>> x=xlsread('membranes') \\
\text{x} = \\
1 & 55 & 73 & 125 \\
2 & 54 & 80 & 123 \\
3 & 55 & 74 & 118 \\
4 & 57 & 77 & 99 \\
5 & 58 & 79 & 123 \\
6 & 52 & 81 & 112 \\
7 & 51 & 80 & 121 \\
8 & 48 & 84 & 132 \\
9 & 61 & 77 & 121 \\
10 & 60 & 72 & 127 \\
\vdots & \vdots & \vdots & \vdots \\
\end{array}
\]

\[
\begin{array}{c}
>> x1=x(:,2); \\
>> x2=x(:,3); \\
>> x3=x(:,4); \\
\end{array}
\]

Results:

- Small pore membranes
  » Mean: too high
  » STD: too high

- Medium pore membranes
  » Mean: too high
  » STD: too low (OK)

- Large pore membranes
  » Mean: too low
  » STD: in range
Exercise

\[
\begin{align*}
\text{muhat} &= 53.9200 \\
\text{sigmahat} &= 4.3004 \\
\text{muci} &= 52.1449, 55.6951 \\
\text{sigmaci} &= 3.3579, 5.9825 \\
\end{align*}
\]

\[
\begin{align*}
\text{muhat} &= 76.7600 \\
\text{sigmahat} &= 3.3823 \\
\text{muci} &= 75.3639, 78.1561 \\
\text{sigmaci} &= 2.6410, 4.7053 \\
\end{align*}
\]
Exercise

\[
\text{>> } [\text{muhat, sigmahat, muci, sigmaci}] = \text{normfit}(x3, 0.05)
\]

\[
\text{muhat} = \\
119.5200
\]

\[
\text{sigmahat} = \\
9.0789
\]

\[
\text{muci} = \\
115.7724 \\
123.2676
\]

\[
\text{sigmaci} = \\
7.0891 \\
12.6301
\]
MATLAB: Statistical Analysis

1. Overview
2. In-class exercise
MATLAB: Statistical Analysis

Overview
Hypothesis Tests

- 17 hypothesis tests available
- ttest – one-sample or paired-sample t-test. Tests if a sample comes from a normal distribution with unknown variance and a specified mean, against the alternative that it does not have that mean.
- vartest – one-sample chi-square variance test. Tests if a sample comes from a normal distribution with specified variance, against the alternative that it comes from a normal distribution with a different variance.
- chi2gof – chi-square goodness-of-fit test. Tests if a sample comes from a specified distribution, against the alternative that it does not come from that distribution.
Mean Hypothesis Test

$$>> h = \text{ttest}(data, m, alpha, tail)$$

- data: vector or matrix of data
- m: expected mean
- alpha: significance level
- Tail = ‘left’ (left handed alternative), ‘right’ (right handed alternative) or ‘both’ (two-sided alternative)
- h = 1 (reject hypothesis) or 0 (accept hypothesis)
- Measurements of polymer molecular weight
  $$\{1.25, 1.36, 1.22, 1.19, 1.33, 1.12, 1.27, 1.27, 1.31, 1.26\}$$
  $$\bar{x} = 1.258 \quad s^2 = 0.0049$$
- Hypothesis: $$\mu_0 = 1.3$$ instead of $$\mu_1 < \mu_0$$

$$>> h = \text{ttest}(x, 1.3, 0.1, 'left')$$

h = 1
Variance Hypothesis Test

>> h = vartest(data,v,alpha,tail)

- data: vector or matrix of data
- v: expected variance
- alpha: significance level
- Tail = ‘left’ (left handed alternative), ‘right’ (right handed alternative) or ‘both’ (two-sided alternative)
- h = 1 (reject hypothesis) or 0 (accept hypothesis)

Measurements of polymer molecular weight:

\[ \bar{x} = 1.258 \quad s^2 = 0.0049 \]

- Hypothesis: \( \sigma^2 = 0.0075 \) and not a different variance

>> h = vartest(x,0.0075,0.1,'both')

h =

0
Linear Regression

>> [k, kint] = regress(y, X, alpha)

• y is a vector containing the dependent variable data

• X is the independent variable data; must contain a vector of ones or the regression will be calculated to pass through the origin

• Confidence level = 1-alpha

• Returns vector of coefficient estimates k with confidence intervals kint
## Linear Regression Example

### Experiment Table

<table>
<thead>
<tr>
<th>Experiment</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactant Concentration</td>
<td>0.1</td>
<td>0.3</td>
<td>0.5</td>
<td>0.7</td>
<td>0.9</td>
<td>1.2</td>
<td>1.5</td>
<td>2.0</td>
</tr>
<tr>
<td>Rate</td>
<td>2.3</td>
<td>5.7</td>
<td>10.7</td>
<td>13.1</td>
<td>18.5</td>
<td>25.4</td>
<td>32.1</td>
<td>45.2</td>
</tr>
</tbody>
</table>

```matlab
>> c = [0.1 0.3 0.5 0.7 0.9 1.2 1.5 2];
>> r  = [2.3 5.6 10.7 13.1 18.5 25.4 32.1 45.2];
>> caug = [ones(length(c), 1), c']
caug =
    1.0000    0.1000
    1.0000    0.3000
    1.0000    0.5000
    1.0000    0.7000
    1.0000    0.9000
    1.0000    1.2000
    1.0000    1.5000
    1.0000    2.0000
```
Linear Regression Example

>> [k, kint] = regress(r’, caug, 0.05);

>> k
   k =
    -1.1847
     22.5524

>> kint
   kint =
    -2.8338  0.4644
     21.0262  24.0787
Correlation Analysis

>> [R,P]=corrcoef(x,y)

- R is a matrix of correlation coefficients calculated from vectors x and y
- The correlation coefficient of interest is located in the off-diagonal entries of the R matrix
- P a matrix of p-values for testing the hypothesis of no correlation. Each p-value is the probability of getting a correlation as large as the observed value by random chance, when the true correlation is zero.
- If P(i,j) is small, say less than 0.05, then the correlation R(i,j) is significant
Correlation Analysis Example

<table>
<thead>
<tr>
<th>Experiment</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen Concentration</td>
<td>0</td>
<td>0.1</td>
<td>0.3</td>
<td>0.5</td>
<td>1.0</td>
<td>1.5</td>
<td>2.0</td>
<td>3.0</td>
</tr>
<tr>
<td>Polymerization rate</td>
<td>9.7</td>
<td>9.2</td>
<td>10.7</td>
<td>10.1</td>
<td>10.5</td>
<td>11.2</td>
<td>10.4</td>
<td>10.8</td>
</tr>
</tbody>
</table>

```matlab
>> h = [0 0.1 0.3 0.5 1 1.5 2 3];
>> p = [9.7 9.2 10.7 10.1 10.5 11.2 10.4 10.8];
>> [R,P] = corrcoef(h,p)
```

R =

```
    1.0000  0.6238
   0.6238  1.0000
```

P =

```
    1.0000  0.0984
   0.0984  1.0000
```

- Accept hypothesis that x and y are uncorrelated at 5% significance level
Response Surface Models

- Example – three inputs \((x_1, x_2, x_3)\) and one output \((y)\)
  - Linear model
    \[
y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3
    \]
  - Linear model with interactions
    \[
y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3
    \]
  - Quadratic model
    \[
y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2
    \]
Response Surface Modeling

- RSTOOL(X,Y,MODEL) opens a GUI for fitting a polynomial response surface for a response variable Y as a function of the multiple predictor variables in X.
- Distinct predictor variables should appear in different columns of X. Y can be a single vector or a matrix, with columns corresponding to multiple responses.
- RSTOOL displays a family of plots, one for each combination of columns in X and Y. 95% global confidence intervals are shown as two red curves.
- MODEL controls the regression model.
  » 'linear' – Constant and linear terms (the default)
  » 'interaction' – Constant, linear, and interaction terms
  » 'quadratic' – Constant, linear, interaction, and squared terms
  » 'purequadratic' – Constant, linear, and squared terms
MATLAB: Statistical Analysis

In-class Exercise
Response Surface Modeling Example

Olefin Polymerization System

Monomer

Comonomer

Purification Train

ZipperClave®
500 ml Reactor
Polymer Reactor Data Regression

- **Input variables**
  - Catalyst and co-catalyst concentrations
  - Monomer and co-monomer concentrations
  - Reactor temperature

- **Output variables**
  - Polymer production rate
  - Copolymer composition
  - 2 molecular weight measures

- **Dataset available in Excel spreadsheet reactordata.xls**
  - 27 experiments with different input combinations
  - Data collected for all 4 outputs
  - Perform analysis only for polymer production rate
Polymer Reactor Data Regression

```matlab
>> data=xlsread('reactordata');
>> size(data)
ans =
    10    27
>> x=data(2:6,:);
>> y=data(7,:);
>> size(x)
ans =
    5    27
>> size(y)
ans =
    1    27
>> rstool(x',y')
```